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User's Guide for Vectorized Code EQUIL for Calculating Equilibrium Chemistry on Control Data STAR-100 Computer

Ajay Kumar, Randolph A. Graves, Jr.,
and K. James Weilmuenster

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Ajay Kumar
Old Dominion University
Norfolk, Virginia

Randolph A. Graves, Jr., and K. James Weilmuenster
Langley Research Center
Hampton, Virginia

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and Space Administration

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SUMMARY

A vectorized code, EQUIL, is developed for calculating the equilibrium chemistry of a reacting gas mixture on the Control Data STAR-100 computer. The code provides species mole fractions, mass fractions, and thermodynamic and transport properties of the mixture for given temperature, pressure, and elemental mass fractions. The code is set up for the e^-, H, He, C, O, N system of elements. In all, 24 chemical species are included.

INTRODUCTION

This report presents a vectorized code, EQUIL, developed for the Control Data STAR-100 computer, which calculates the equilibrium chemistry of a reacting gas mixture. Only gaseous species are considered. The code (see appendix A) provides species mole fractions, mass fractions, and thermodynamic and transport properties of the mixture for given temperature, pressure, and elemental mass fractions. It can be used as a subprogram to a flow-field code. The code is set up for the e^-, H, He, C, O, N system of elements. In all, 24 species are included. The method given in references 1 and 2 is used in the present code for calculating the equilibrium composition. It uses the free-energy-minimization technique in which the method of steepest descent is utilized. Thermodynamic properties, thermal conductivity, and viscosity of each input species are evaluated by polynomial expressions. The coefficients for these polynomials are prescribed input to the code. The mixture transport properties are determined by using the semiempirical relation of Wilke (ref. 3).

The code is set up for calculating the equilibrium chemistry over 500 mesh points. The number of mesh points can be varied by suitably changing the code dimensions. The system of elements and species considered in this code can also be changed by suitably modifying the input data.

SYMBOLS

$a_1,a_2,\ldots,a_7$ coefficients in approximating polynomials for c_p, H, and F

b_1,b_2,b_3 coefficients in approximating polynomial for μ

c_1,c_2 coefficients in approximating polynomial for k

c_p specific heat at constant pressure

F free energy

H enthalpy

k thermal conductivity

R universal gas constant

T temperature

μ viscosity

PROGRAM INPUT

Most of the data input to the EQUIL code is by punched cards. The detailed input information is presented in the following section.

Chemistry and Transport Model Input

The elements and species in the mixture are input through NAMELIST THERMO, which is described in table I. Thermodynamic properties (refs. 4 to 7), thermal conductivity, and viscosity of each input species are represented by approximating polynomials. The thermodynamic data are input by cards as follows. There are eight cards for each atomic, molecular, or ionic species:

Card 1 (Format (A6, 4X, 6F5.0)): Field 1 contains the alphanumeric identifier for the ith species SYMB(I), which is right justified in columns 1 to 6. Fields 2 to 7 (columns 11 to 15, 16 to 20, etc.) contain the array AA(I,J) for J = 1 to NE, which specifies the number of atoms of each element in the species (see table II). The order must correspond to the order of input of the MWEL array. For example, card 1 for species NO^+ would be

NO^+ -1. 0. 0. 0. 1. 1.

Cards 2 and 3 (Format (5E14.6)) contain the seven constants a_1 to a_7 used in the polynomials for calculating the specific heat, enthalpy, and free energy of each species in the temperature range from 300 K to 1000 K. These polynomials are

$$\frac{c_p}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$\frac{H}{RT} = a_1 + a_2\frac{T}{2} + a_3\frac{T^2}{3} + a_4\frac{T^3}{4} + a_5\frac{T^4}{5} + \frac{a_6}{T}$$

$$\frac{F}{RT} = a_1(1 - \ln T) - a_2\frac{T}{2} - a_3\frac{T^2}{6} - a_4\frac{T^3}{12} - a_5\frac{T^4}{20} + \frac{a_6}{T} + a_7$$

Columns 29 to 80 of card 2 may be used for identification purposes.

Cards 4 and 5 (Format (5E14.6)) contain constants a_1 to a_7 for the thermodynamic data in the temperature range from 1000 K to 6000 K.

Cards 6 and 7 (Format (5E14.6)) contain constants a_1 to a_7 for the thermodynamic data in the temperature range above 6000 K.

Card 8 (Format (5E14.6)) contains the constants b_1, b_2, b_3, c_1, and c_2 in the approximating polynomials for viscosity and thermal conductivity, which are

$$\mu = b_1 + b_2T + b_3T^2$$

$$k = c_1 + c_2$$

where T is in K, μ is in lbm/ft-sec, and k is in Btu/ft-sec-^{o}R.*

Coefficients for the species used in this code are given in appendix B.

The elements are input in the order e^-, H, He, C, O, and N. The order of species input is shown in table II. The species composition is described using the AA(24,6) array in table II. For example, AA(i,2) defines the number of hydrogen atoms in species i, and AA(i,4) defines the number of carbon atoms in species i. If species i is a positive ion, then AA(i,1) is -1.

Temperature, Pressure, and Elemental Mass Fractions Input

The code is set to calculate the equilibrium chemistry at 500 mesh points. This can be varied by changing the dimensions of various variables. The temperature, pressure, and elemental mass fractions at all the mesh points are input to the code through vectors T(500), P(500), and CL(500,6). The temperature is in kelvins and pressure is in atmospheres. The code requires that at least one element of the temperature vector be in each temperature range used to calculate the thermodynamic properties in subroutine THERMO. As an example, the present code is set to use only two temperature ranges, $1000\ K < T < 6000\ K$ and $T > 6000$ K. There is a transition range from 5500 K to 6500 K to assure smooth transition from one temperature range to another. The temperature vector should have at least one element less than 5500 K, at least one element between 5500 K and 6500 K, and at least one element above 6500 K.

The vector CL(500,1) is an elemental array and, for the present setup, represents the charge balance, which is zero. However, the solution procedure does not allow zero values for an elemental array; therefore, the "electron" elemental array is set to an arbitrary small number. In this code, CL(500,1) is taken as 1.E-10 for all cases. No element should have zero mass fraction. For cases where the mixture does not include a particular element, the mass fraction for that element can be prescribed as an arbitrary small number.

---

*1 lbm/ft-sec = 1.488 Pa-sec; 1 Btu/ft-sec-^{o}R = 6226.5 W/m-K.

In addition to the aforementioned input quantities, a criterion for the convergence of the calculation procedure is required. The convergence criterion is as follows:

$$CRIT = \sum_{i=1}^{N} |X_i - Y_i| < 1.E-6$$

Here, the values of X_i are the species mole numbers for the current iteration, and the values of Y_i are the species mole numbers for the previous iteration. Thus, when the sum of the absolute values of the changes in the mole numbers for all the species is less than 1.E-6 from one iteration to the next, the calculation is terminated. The value of CRIT can be changed if necessary.

CODE STRUCTURE

Code EQUIL has a main program in which the quantities such as temperature, pressure, and elemental mass fractions are prescribed at all the mesh points. The value of CRIT is also input here. In addition to the main program, there are six subroutines.

Subroutine READ reads the NAMELIST THERMO and thermodynamic and transport data for various species. Subroutine THERMO calculates the thermodynamic properties of various species at all the mesh points. Subroutines CHEQ, MINENG, and EQSOL use the method of steepest descent to minimize the free energy. An initial assumption is made on the mole numbers of various species, and then an iterative procedure is followed to find the set of mole numbers of various species which minimizes the free energy.

Knowing the right mole numbers of various species, the subroutine CHEQ then calculates the mixture molecular weight, mole fractions, and the enthalpy of the mixture. Subroutine TP calculates the mixture specific heat, thermal conductivity, viscosity, and Prandtl number.

Finally, the main program EQUIL converts the mixture viscosity, conductivity, and specific heat to SI units. The species mass fractions are also obtained here. The printed output includes the mole fractions of various species, and the enthalpy, specific heat, viscosity, conductivity, Prandtl number, and molecular weight of the mixture.

LIST OF VARIABLES

CIS	Species mass fraction
CL	Elemental mass fraction
COND	Thermal conductivity of mixture
CONDI	Thermal conductivity of individual species

CP	Specific heat of mixture
CPI	Specific heat of individual species
CRIT	Convergence criterion
FORT	Free energy of individual species
HI	Enthalpy of individual species
KTEST	A parameter equal to either zero or one
MOLEF	Mole fraction of species
MW	Molecular weight of species
MWEL	Molecular weight of element
P	Pressure
SH	Enthalpy of mixture
SIG	Prandtl number of mixture
T	Temperature
VIS	Viscosity of mixture
VISI	Viscosity of individual species
WMIX	Molecular weight of mixture
Y	Mole number of species in current iteration
YI1	Mole number of species in previous iteration used to start a new iteration for KTEST = 1

SAMPLE CALCULATIONS

Two sample calculations are presented here. The first example is for a mixture consisting mainly of e^-, H, He, C, and O elements. The input temperature, pressure, and elemental mass fractions are listed below:

T(1;100) = 4000.

T(101;100) = 6000.

T(201;300) = 12570.

P(1;500) = 6.3549

CL(1,1;500) = 1.E-10

CL(1,3;500) = 0.1008

CL(1,4;500) = 0.4518

CL(1,5;500) = 0.02443

CL(1,6;500) = 5.E-6

CL(1,2;500) = 1. - (Sum of other five elemental mass fractions)

The mass fraction for the sixth element, nitrogen, was prescribed as a very small number. It took 24 iterations for the solution to converge. The actual computing time on the Control Data STAR-100 computer for this example was 5.3 seconds. The output for this example is given in table III.

The second example is for air. For this example, the elemental mass fractions for H, He, and C were prescribed as small numbers. The input temperature, pressure, and elemental mass fractions are as follows:

T(1;100) = 7000.

T(101;100) = 6000.

T(201;300) = 3991.17

P(1;500) = 1.146

CL(1,1;500) = 1.E-10

CL(1,2;500) = 5.E-6

CL(1,3;500) = 5.E-6

CL(1,4;500) = 5.E-6

CL(1,5;500) = 0.233

CL(1,6;500) = 1. - (Sum of other five elemental mass fractions)

It took 26 iterations and 6.2 seconds actual computing time for the solution to converge. The output for this example is given in table IV.

In these examples, the input conditions for the first 100 mesh points, for the next 100 mesh points, and for the last 300 mesh points were the same; consequently, tables III and IV give the results only at mesh points 1, 101, and 201.

CONCLUDING REMARKS

The code presented in appendix A calculates the enthalpy of the mixture for given temperature, pressure, and elemental mass fractions. However, in most flow-field calculations, it is the temperature which is to be calculated for given enthalpy and pressure. To use this code for such calculations, an iterative technique can be used in which a temperature is assumed initially. For this temperature, the enthalpy of the mixture is obtained from EQUIL. The temperature is then changed using the Newton-Raphson technique until the enthalpy of the mixture is obtained within desired accuracy to the initially known value. This iterative technique can be incorporated in the main program EQUIL, and only subroutines THERMO and CHEQ are required to be put in the iterative loop.

To save significantly on time for such calculations, a parameter KTEST is used. For the initial guess of temperature, KTEST is set equal to zero and for subsequent guesses, KTEST is set equal to one. When KTEST = 0, the subroutine CHEQ starts with a very crude approximation of species mole numbers. For KTEST = 1, mole numbers calculated in the previous iteration are taken as the starting approximation and the solution converges in fewer iterations.

Langley Research Center
National Aeronautics and Space Administration
Hampton, VA 23665
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APPENDIX A

PROGRAM LISTING

The computational program EQUIL is listed in this appendix in Control Data STAR-100 FORTRAN language 1.4 (an extension of ANSI FORTRAN for the Control Data STAR-100 computer). This program consists of one main program and six subroutines.

```
      PROGRAM EQUIL(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION CIS(500,24)
      COMMON/E1/T(500),P(500),WMIX(500),CL(500,6),SH(500)
      COMMON/E2/HI(500,24),MOLEF(500,24),CPI(500,24)
      COMMON/E4/MW(24),SYMB(24),AA(24,6),MWEL(6),AAA(500,24,6)
      COMMON/E8/NE,NS
      COMMON/E14/VIS(500),COND(500),SIG(500),CP(500)
      COMMON/E15/RR,CRIT,RCRIT,MNS,MMM,MNE,MNE1,MX
      COMMON/E16/ENT(500,24),CPI1(500,24)
      EQUIVALENCE (CIS(1,1),ENT(1,1))
      REAL MW,MWEL,MOLEF
      RR=1.987
      CRIT=1.E-6
      RCRIT=.1*CRIT
      M1=500
C     T IS IN DEGREE K AND P IS IN ATM.
      T(1:100)=4000.
      T(101:100)=6000.
      T(201:300)=12570.
      P(1:M1)=6.3549
C     THE ELEMENTS ARE IN THE ORDER OF E-,H,HE,C,O AND N.
      CL(1,1:M1)=1.E-10
      CL(1,2:M1)=.4229649999
      CL(1,3:M1)=.1008
      CL(1,4:M1)=.4518
      CL(1,5:M1)=.02443
      CL(1,6:M1)=5.E-6
      CALL READ(M1)
      MNS=M1*NS
      MMM=NE+1
      MNE=M1*NE
      MNE1=MMM*M1
      MX=MMM*MMM*M1
      CALL THERMO(M1)
      KTEST=0
      CALL CHEQ(KTEST,M1)
      CALL TP(M1)
      DO 10 I=1,NS
C     CIS IS THE MASS FRACTION OF SPECIE I. HI IS IN J/KG.
      CW=MW(I)
      CW1=4184./CW
      CIS(1,I:M1)=MOLEF(1,I:M1)*CW/WMIX(1:M1)
   10 HI(1,I:M1)=HI(1,I:M1)*CW1
C     HERE SH IS IN J/KG, CP IS IN J/KG K, VIS IS IN N SEC/M2, COND IS
C     IN W/M K.
      SH(1:M1)=SH(1:M1)*4184.
```

```
      CP(1:M1)=CP(1:M1)*4184./WMIX(1:M1)
      VIS(1:M1)=0.1*VIS(1:M1)
      COND(1:M1)=418.4384*COND(1:M1)
C     THE SPECIES ARE IN THE ORDER OF E-,H,H2,H+,HE,HE+,C,C2,C3,C+,C2H,
C     C2H2,C3H,C4H,O,O2,O+,CO,CO2,N,N2,N+,NO,NO+
      WRITE(6,100)
      WRITE(6,130)(M,MOLEF(M,1),MOLEF(M,2),MOLEF(M,3),MOLEF(M,4),MOLEF(M
     1,5),MOLEF(M,6),M=1,M1,100)
      WRITE(6,120)
      WRITE(6,130)(M,MOLEF(M,7),MOLEF(M,8),MOLEF(M,9),MOLEF(M,10),
     1MOLEF(M,11),MOLEF(M,12),M=1,M1,100)
      WRITE(6,140)
      WRITE(6,130)(M,MOLEF(M,13),MOLEF(M,14),MOLEF(M,15),MOLEF(M,16),
     1MOLEF(M,17),MOLEF(M,18),M=1,M1,100)
      WRITE(6,160)
      WRITE(6,130)(M,MOLEF(M,19),MOLEF(M,20),MOLEF(M,21),MOLEF(M,22),
     1MOLEF(M,23),MOLEF(M,24),M=1,M1,100)
      WRITE(6,150)
      WRITE(6,130)(M,SH(M),CP(M),VIS(M),COND(M),SIG(M),WMIX(M),M=1,M1,
     1100)
  100 FORMAT(/,4X,'M',11X,'XE',13X,'XH',13X,'XH2',12X,'XH+',12X,'XHE',
     111X,'XHE+',/)
  120 FORMAT(/,4X,'M',11X,'XC',12X,'XC2',12X,'XC3',12X,'XC+',12X,'XC2H',
     111X,'XC2H2',/)
  130 FORMAT(2X,I4,2X,6E15.5)
  140 FORMAT(/,4X,'M',11X,'XC3H',11X,'XC4H',11X,'XO',13X,'XO2',12X,'XO+'
     111X,'XCO',/)
  160 FORMAT(/,4X,'M',11X,'XCO2',11X,'XN',12X,'XN2',12X,'XN+',12X,'XNO',
     112X,'XNO+',/)
  150 FORMAT(/,4X,'M',11X,'SH',12X,'CP',13X,'VIS',12X,'COND',11X,'SIG',
     111X,'WMIX',/)
      STOP
      END
      SUBROUTINE READ(M1)
      COMMON/E3/AI(24,3),BI(24,3),CI(24,3),DI(24,3),EI(24,3),FI(24,3),
     1GI(24,3)
      COMMON/E4/MW(24),SYMB(24),AA(24,6),MWEL(6),AAA(500,24,6)
      COMMON/E8/NE,NS
      COMMON/E9/XMA(24),XMB(24),XMC(24),XKA(24),XKB(24)
      DIMENSION ILW(9),ILWP(6)
      REAL MW,MWEL
      DATA ILW/5H   SI,5H    F,5H    O,5H    N,5H    C,5H   HE,
     15H    H,5H   E-,5H      /
      NAMELIST/THERMO/       MW,MWEL,NE,NS
C  INPUT PROBLEM NAMELISTS
   20 READ(5,THERMO)
```

```
      WRITE(6,THERMO)
      DO 60 I=1,NS
      READ(5,901) SYMB(I),(AA(I,J),J=1,NE)
      DO 55 J= 1,3
 55   READ(5,902)AI(I,J),BI(I,J),CI(I,J),DI(I,J),EI(I,J),FI(I,J),GI(I,J)
      READ(5,902)XMA(I),XMB(I),XMC(I),XKA(I),XKB(I)
 60   CONTINUE
C  THERMOCHEMICAL PROPERTIES
      WRITE(6,919)
      DO 120 I=1,NS
      WRITE(6,920) SYMB(I),(AI(I,J),BI(I,J),CI(I,J),DI(I,J),EI(I,J),
     .                          FI(I,J),GI(I,J),J= 1,3)
 120  CONTINUE
  122 WRITE(6,921)
      DO 130 I=1,NS
      WRITE(6,922) SYMB(I),XMA(I),XMB(I),XMC(I),XKA(I),XKB(I)
 130  CONTINUE
C  SPECIES/ELEMENTAL COMPOSITION MATRIX
      DO 135 I=1,NE
      ILWP(I)=ILW(1)
      IF(MWEL(I).LT.27.) ILWP(I)=ILW(2)
      IF(MWEL(I).LT.17.) ILWP(I)=ILW(3)
      IF(MWEL(I).LT.15.) ILWP(I)=ILW(4)
      IF(MWEL(I).LT.13.) ILWP(I)=ILW(5)
      IF(MWEL(I).LT.4.1) ILWP(I)=ILW(6)
      IF(MWEL(I).LT.1.1) ILWP(I)=ILW(7)
      IF(MWEL(I).LT.0.1) ILWP(I)=ILW(8)
      IF(MWEL(I).EQ.0.0) ILWP(I)=ILW(9)
 135  CONTINUE
      WRITE(6,923) ILWP
      DO 140 I=1,NS
      DO 137 J=1,NE
      IF(AA(I,J).EQ.0.) AA(I,J)=0.
 137  CONTINUE
      WRITE(6,924) SYMB(I),(AA(I,J),J=1,NE)
 140  CONTINUE
 901  FORMAT(A6,4X,6F5.0)
 902  FORMAT(5E14.6)
 919  FORMAT(1H1,34X,'THERMOPHYSICAL PROPERTIES - CURVE FIT COEFFICIENTS
     .'//46X,'(1) THERMODYNAMIC PROPERTIES'//4X,'SPECIES',11X,'A',14X,
     .'B',14X,'C',14X,'D',14X,'E',14X,'F',14X,'G'/)
 920  FORMAT(1H0,5X,A6,3X,7E15.6,' T= 300K'/15X,7E15.6,' T=1000K'/15X,
     .  7E15.6,' T=6000K')
 921  FORMAT(1H0/4X,'SPECIES',30X,'VISCOSITY',28X,1H*,12X,'CONDUCTIVITY'
     ./)
 922  FORMAT(1H ,4X,A6,4X,3E20.6,3X,1H*,E16.6,E20.6)
```

APPENDIX A

```
923   FORMAT(1H0//49X,'ELEMENTAL PARTICLES TABLE'/42X,' SPECIES ',6A5)
924   FORMAT(1H ,43X,A6,1X,6F5.0)
      NSNEM1=NS*NE*M1
      AAA(1,1,1;NSNEM1)=0.
      DO 110 I=1,M1
      DO 110 J=1,NS
      DO 110 K=1,NE
110   AAA(I,J,K)=AA(J,K)
      RETURN
      END
      SUBROUTINE THERMO(M1)
C  FREE ENERGY, ENTHALPY, AND SPECIFIC HEAT BY APPROXIMATING POLYNOMIALS
      DIMENSION BG(500)
      COMMON/E1/T(500),P(500),WMIX(500),CL(500,6),SH(500)
      COMMON/E2/HI(500,24),MOLEF(500,24),CPI(500,24)
      COMMON/E3/AI(24,3),BI(24,3),CI(24,3),DI(24,3),EI(24,3),FI(24,3),
     1GI(24,3)
      COMMON/E5/FORT(500,24),Y(500,24),X(500,24),YBAR(500)
      COMMON/E8/NE,NS
      COMMON/E12/A9(500),A10(500),A13(500),AA1(500),AA2(500),TV1(500),
     1TV2(500)
      COMMON/E15/RR,CRIT,RCRIT,MNS,MMM,MNE,MNE1,MX
      COMMON/E16/ENT(500,24),CPI1(500,24)
      DESCRIPTOR DA1,DA9
      BIT BG
      REAL MOLEF
C     COEFFICINTS ARE INPUT FOR THREE TEMPERATURE RANGES. (1) 300K TO
C     1000K, (2) 1000K TO 6000K, AND (3) 6000K TO 15000K. K AND L
C     DENOTES THE SET OF COEFFICIENTS THAT ARE BEING USED.  COMBINE TO
C     ASSURE SMOOTH TRANSITION BETWEEN EACH OF THE THREE TEMPERATURE
C     INTERVALS. T IS GENERALLY GREATER THAN 6500K.
C     T VECTOR SHOULD CONTAIN ATLEAST ONE ELEMENT LESS THAN 5500K,ONE
C     ELEMENT BETWEEN 55005 AND 6500K, AND ONE ELEMENT ABOVE 6500K.
      BG(1;M1)=T(1;M1).LE.6500.
      ASSIGN DA9,A9(1;M1)
      DA9=Q8VCMPRS(T(1;M1),BG(1;M1);DA9)
      L1=Q8SLEN(DA9)
      BG(1;L1)=A9(1;L1).LE.5500.
      ASSIGN DA1,A10(1;M1)
      DA1=Q8VCMPRS(A9(1;L1),BG(1;L1);DA1)
      L2=Q8SLEN(DA1)
      AA1(1;L2)=DA1*DA1
      AA2(1;L2)=DA1*AA1(1;L2)
      A13(1;L2)=AA1(1;L2)*AA1(1;L2)
      TV2(1;L2)=VALOG(DA1;TV2(1;L2))
      TV2(1;L2)=1.-TV2(1;L2)
```

```
      DO 10 I=1,NS
      CPI(1,I;L2)=RR*(AI(I,2)+BI(I,2)*DA1+CI(I,2)*AA1(1:L2)+DI(I,2)*AA2(
     11;L2)+EI(I,2)*A13(1:L2))
      FORT(1,I:L2)=AI(I,2)*TV2(1:L2)-.5*BI(I,2)*DA1-CI(I,2)*AA1(1:L2)/6.
     1-DI(I,2)*AA2(1:L2)/12.-EI(I,2)*0.05*A13(1:L2)+FI(I,2)/DA1-GI(I,2)
      ENT(1,I:L2)=RR*DA1*(AI(I,2)+.5*BI(I,2)*DA1+CI(I,2)*AA1(1:L2)/3.+
     1DI(I,2)*AA2(1:L2)/4.+EI(I,2)*A13(1:L2)/5.+FI(I,2)/DA1)
10    CONTINUE
      BG(1:L1)=A9(1:L1).GT.5500.
      DA1=Q8VCMPRS(A9(1:L1),BG(1:L1);DA1)
      L3=Q8SLEN(DA1)
      AA1(1:L3)=DA1*DA1
      AA2(1:L3)=DA1*AA1(1:L3)
      A13(1:L3)=AA1(1:L3)*AA1(1:L3)
      TV2(1:L3)=VALOG(DA1;TV2(1:L3))
      TV2(1:L3)=1.-TV2(1:L3)
      DO 20 I=1,NS
      TV1(1:L3)=RR*((6.5-.001*DA1)*(AI(I,2)+BI(I,2)*DA1+CI(I,2)*AA1(1:L3
     1)+DI(I,2)*AA2(1:L3)+EI(I,2)*A13(1:L3))+(.001*DA1-5.5)*(AI(I,3)+BI(
     2I,3)*DA1+CI(I,3)*AA1(1:L3)+DI(I,3)*AA2(1:L3)+EI(I,3)*A13(1:L3)))
      CPI1(1,I:L1)=Q8VMERG(TV1(1:L3),CPI(1,I:L2),BG(1:L1);CPI1(1,I:L1))
      TV1(1:L3)=(6.5-.001*DA1)*(AI(I,2)*TV2(1:L3)-.5*BI(I,2)*DA1-CI(I,2)
     1*AA1(1:L3)/6.-DI(I,2)*AA2(1:L3)/12.-EI(I,2)*.05*A13(1:L3)+FI(I,2)/
     2DA1-GI(I,2))+(.001*DA1-5.5)*(AI(I,3)*TV2(1:L3)-0.5*BI(I,3)*DA1-CI(
     3I,3)*AA1(1:L3)/6.-DI(I,3)*AA2(1:L3)/12.-EI(I,3)*.05*A13(1:L3)+
     4FI(I,3)/DA1-GI(I,3))
      HI(1,I:L1)=Q8VMERG(TV1(1:L3),FORT(1,I:L2),BG(1:L1);HI(1,I:L1))
      TV1(1:L3)=RR*DA1*((6.5-.001*DA1)*(AI(I,2)+.5*BI(I,2)*DA1+CI(I,2)*
     1AA1(1:L3)/3.+DI(I,2)*AA2(1:L3)/4.+EI(I,2)*A13(1:L3)/5.+FI(I,2)/DA1
     2)+(.001*DA1-5.5)*(AI(I,3)+.5*BI(I,3)*DA1+CI(I,3)*AA1(1:L3)/3.+DI(I
     3,3)*AA2(1:L3)/4.+EI(I,3)*A13(1:L3)/5.+FI(I,3)/DA1))
      MOLEF(1,I:L1)=Q8VMERG(TV1(1:L3),ENT(1,I:L2),BG(1:L1);MOLEF(1,I:L1)
     1)
20    CONTINUE
      BG(1:M1)=T(1:M1).GT.6500.
      DA1=Q8VCMPRS(T(1:M1),BG(1:M1);DA1)
      L2=Q8SLEN(DA1)
      AA1(1:L2)=DA1*DA1
      AA2(1:L2)=DA1*AA1(1:L2)
      A13(1:L2)=AA1(1:L2)*AA1(1:L2)
      TV2(1:L2)=VALOG(DA1;TV2(1:L2))
      TV2(1:L2)=1.-TV2(1:L2)
      DO 30 I=1,NS
      TV1(1:L2)=RR*(AI(I,3)+BI(I,3)*DA1+CI(I,3)*AA1(1:L2)+DI(I,3)*AA2(1;
     1L2)+EI(I,3)*A13(1:L2))
      CPI(1,I:M1)=Q8VMERG(TV1(1:L2),CPI1(1,I:L1),BG(1:M1);CPI(1,I:M1))
```

```
      TV1(1;L2)=AI(I,3)*TV2(1;L2)-.5*BI(I,3)*DA1-CI(I,3)*AA1(1;L2)/6.-DI
     1(I,3)*AA2(1;L2)/12.-EI(I,3)*0.05*A13(1;L2)+FI(I,3)/DA1-GI(I,3)
      FORT(1,I;M1)=Q8VMERG(TV1(1;L2),HI(1,I;L1),BG(1;M1);FORT(1,I;M1))
      TV1(1;L2)=RR*DA1*(AI(I,3)+.5*BI(I,3)*DA1+CI(I,3)*AA1(1;L2)/3.+DI(I
     1,3)*AA2(1;L2)/4.+EI(I,3)*A13(1;L2)/5.+FI(I,3)/DA1)
      ENT(1,I;M1)=Q8VMERG(TV1(1;L2),MOLEF(1,I;L1),BG(1;M1);ENT(1,I;M1))
 30   CONTINUE
      TV1(1;M1)=VALOG(P(1;M1);TV1(1;M1))
      DO 50 I=1,NS
 50   FORT(1,I;M1)=FORT(1,I;M1)+TV1(1;M1)
      HI(1,1;NS*M1)=ENT(1,1;NS*M1)
      RETURN
      END
      SUBROUTINE CHEQ(KTEST,M1)
C     CHEMICAL EQUILIBRIUM OF MULTIPHASE SYSTEMS BASED ON THE PRINCIPLE
C     OF MINIMIZATION OF THE FREE ENERGY OF THE MIXTURE
C   THE CONDENSED SPECIES OPTION IS NOT CURRENTLY IMPLEMENTED.
      COMMON/E1/T(500),P(500),WMIX(500),CL(500,6),SH(500)
      COMMON/E2/HI(500,24),MOLEF(500,24),CPI(500,24)
      COMMON/E4/MW(24),SYMB(24),AA(24,6),MWEL(6),AAA(500,24,6)
      COMMON/E5/FORT(500,24),Y(500,24),X(500,24),YBAR(500)
      COMMON/E6/YI1(500,24)
      COMMON/E8/NE,NS
      COMMON/E10/SKIP(500)
      COMMON/E11/CONV(500),XLAMBD(500),DELT(500,24),F(500,24),DEBAR(500)
     1,HALL(500),DEDL(500)
      COMMON/E12/A9(500),A10(500),A13(500),AA1(500),AA2(500),TV1(500),
     1TV2(500)
      COMMON/E15/RR,CRIT,RCRIT,MNS,MMM,MNE,MNE1,MX
      DIMENSION BIG(500),WMIX1(500)
      EQUIVALENCE (WMIX1(1),A9(1))
      BIT BIG
      REAL MW,MWEL,MOLEF
      NT=0
      SKIP(1;M1)=0.
C     IF KTEST EQ 1 USE MOLE NUMBERS COMPUTED PREVIOUSLLY FOR THIS
C    STATION AS INITIAL GUESS.
C    OTHERWISE,ESTIMATE SPECIES MOLE NUMBERS FROM ELEMENT
C    MASS FRACTIONS.
      IF(KTEST.EQ.1)GO TO 48
C    STARTING ASSUMPTION - ATOMS ONLY, NO COMPOUNDS
      Y(1,1;MNS)=1.E-7
      Y(1,1;M1)=CL(1,1;M1)/MWEL(1)
      Y(1,2;M1)=CL(1,2;M1)/MWEL(2)
      Y(1,5;M1)=CL(1,3;M1)/MWEL(3)
      Y(1,7;M1)=CL(1,4;M1)/MWEL(4)
```

```
      Y(1,15:M1)=CL(1,5:M1)/MWEL(5)
      Y(1,20:M1)=CL(1,6:M1)/MWEL(6)
      GO TO 50
 48   CONTINUE
      DO 42 I=1,NS
 42   Y(1,I:M1)=YI1(1,I:M1)
 50   CONTINUE
C  FREE ENERGY MINIMIZATION BY STEEPEST DESCENT
 60   CONTINUE
      NT=NT+1
      CALL MINENG(NS,NE,M1)
C  LAMBDA AND DIRECTIONAL DERIVATIVE (DEDL), AND CONVERGENCE TEST
      XLAMBD(1:M1)=1.
      DELT(1,1:MNS)=X(1,1:MNS)-Y(1,1:MNS)
      DO 100 M=1,M1
      IF(SKIP(M).EQ.1.)GO TO 105
      IF(NT.LE.8)GO TO 107
      IF(NT.GE.17.AND.NT.LE.22)GO TO 107
      DO 101 I=1,NS
      IF(DELT(M,I).GE.0.)GO TO 101
      IF(YI1(M,I).LT.1.E-7)GO TO 102
      XLAM=-Y(M,I)/DELT(M,I)
      IF(XLAM.GE.XLAMBD(M))GO TO 101
      XLAMBD(M)=0.9999999*XLAM
      GO TO 101
 102  DELT(M,I)=0.
 101  CONTINUE
      GO TO 100
 107  DO 103 I=1,NS
      IF(DELT(M,I).GE.0.)GO TO 103
      XLAM=-Y(M,I)/DELT(M,I)
      IF(XLAM.GE.XLAMBD(M))GO TO 103
      XLAMBD(M)=0.9999999*XLAM
 103  CONTINUE
      GO TO 100
 105  DO 106 J=1,NS
 106  DELT(M,J)=0.
 100  CONTINUE
C  DERIVATIVE FOR GASEOUS SPECIES.
      F(1,1:MNS)=VABS(DELT(1,1:MNS):F(1,1:MNS))
      CONV(1:M1)=0.
      DEBAR(1:M1)=0.
      DO 110 I=1,NS
      CONV(1:M1)=F(1,I:M1)+CONV(1:M1)
 110  DEBAR(1:M1)=DELT(1,I:M1)+DEBAR(1:M1)
      NTRIES=0
```

```
 120  CONTINUE
      HALL(1:M1)=1./(YBAR(1:M1)+XLAMBD(1:M1)*DEBAR(1:M1))
      NTRIES=NTRIES+1
      DO 130 I=1,NS
 130  F(1,I:M1)=(Y(1,I:M1)+XLAMBD(1:M1)*DELT(1,I:M1))*HALL(1:M1)
      F(1,1:MNS)=VALOG(F(1,1:MNS):F(1,1:MNS))
      DFDL(1:M1)=0.
      DO 140 I=1,NS
      F(1,I:M1)=DELT(1,I:M1)*(FORT(1,I:M1)+F(1,I:M1))
 140  DFDL(1:M1)=DFDL(1:M1)+F(1,I:M1)
C   IF DFDL < 0, WE ARE GOING THE RIGHT WAY ON FREE ENERGY SURFACE.
C   IF NOT, REDUCE LAMBDA AND TRY AGAIN...
      BIG(1:M1)=SKIP(1:M1).EQ.1.
      DFDL(1:M1)=Q8VCTRL(1.E-10,BIG(1:M1):DFDL(1:M1))
      BIG(1:M1)=DFDL(1:M1).GE.1.E-9
      HALL(1:M1)=.75*XLAMBD(1:M1)
      XLAMBD(1:M1)=Q8VCTRL(HALL(1:M1),BIG(1:M1):XLAMBD(1:M1))
      II=Q8SGE(DFDL(1:M1),1.E-9)
      IF(II.EQ.M1)GO TO 200
      IF(NTRIES.GT.16)GO TO 600
      GO TO 120
 200  CONTINUE
C   NEW MOLE FRACTIONS
      HALL(1:M1)=VABS(DFDL(1:M1);HALL(1:M1))
      BIG(1:M1)=HALL(1:M1).LT.1.E-9
      CONV(1:M1)=Q8VCTRL(RCRIT,BIG(1:M1):CONV(1:M1))
      BIG(1:M1)=CONV(1:M1).LE.CRIT
      XLAMBD(1:M1)=Q8VCTRL(0.,BIG(1:M1):XLAMBD(1:M1))
      SKIP(1:M1)=Q8VCTRL(1.,BIG(1:M1):SKIP(1:M1))
      II=Q8SGE(CONV(1:M1),CRIT)
      IF(II.EQ.M1)GO TO 600
      DO 220 I=1,NS
 220  Y(1,I:M1)=Y(1,I:M1)+XLAMBD(1:M1)*DELT(1,I:M1)
      IF(NT.LT.50)GO TO 500
      WRITE(6,231)
 231  FORMAT(/1X,'NO. OF ITERATIONS EXCEED  50'/)
      DO 350 M=1,M1
      IF(SKIP(M).EQ.1.)GO TO 350
      WRITE(6,300)M,P(M),T(M),DFDL(M),CONV(M),XLAMBD(M)
 350  CONTINUE
 300  FORMAT(1X,             I4,5X,'P=',F12.5,5X,'T=',F13.5,5X,'DFDL=',
     1E12.5,3X,'CONV=',E12.5,3X,'XLAMBD=',E11.5)
      GO TO 600
 500  GO TO 60
 600  CONTINUE
      WRITE(6,70)NT
```

```
 70    FORMAT(/,10X,'NO. OF ITERATIONS=',I4,/)
       YI1(1,1:MNS)=Y(1,1:MNS)
       SH(1:M1)=0.
       WMIX1(1:M1)=0.
       TV2(1:M1)=0.
       DO 10 I=1,NS
       CW=MW(I)
       WMIX1(1:M1)=WMIX1(1:M1)+YI1(1,I:M1)
 10    TV2(1:M1)=TV2(1:M1)+YI1(1,I:M1)*CW
C   MOLECULAR WEIGHT OF EQUILIBRIUM MIXTURE
       WMIX(1:M1)=TV2(1:M1)/WMIX1(1:M1)
C      ENTHALPY OF EQUIL. MIXTURE IN CAL/MOL. DIVIDE BY MIXTURE MOL. WT.
C      TO GET IN CAL/GM.
C      1 CAL/GM = 4184 J/KG.
       DO 20 I=1,NS
       SH(1:M1)=SH(1:M1)+HI(1,I:M1)*YI1(1,I:M1)
 20    MOLEF(1,I:M1)=YI1(1,I:M1)/WMIX1(1:M1)
       SH(1:M1)=SH(1:M1)/TV2(1:M1)
       RETURN
       END
       SUBROUTINE MINENG(NS,NE,M1)
C   FIT N-DIMENSIONAL PARABOLA TO POINT IN FREE-ENERGY SPACE, WHERE
C   N IS NUMBER OF ELEMENTS IN SYSTEM.
       DIMENSION DELTA(500,24,6),F(500,24),DELT(500,24),BUM(500),
      1XYBAR(500),R1(500,7,7)
       COMMON/E4/MW(24),SYMB(24),AA(24,6),MWEL(6),AAA(500,24,6)
       COMMON/E5/FORT(500,24),Y(500,24),X(500,24),YBAR(500)
       COMMON/E6/YI1(500,24)
       COMMON/E7/A1(500,7,7),BB1(500,7)
       COMMON/E10/SKIP(500)
       COMMON/E15/RR,CRIT,RCRIT,MNS,MMM,MNE,MNE1,MX
       COMMON/E16/ENT(500,24),CPI1(500,24)
       EQUIVALENCE (F(1,1),ENT(1,1)),(DELT(1,1),CPI1(1,1))
       YBAR(1:M1)=0.
       DO 100 I=1,NS
 100   YBAR(1:M1)=YBAR(1:M1)+Y(1,I:M1)
C   SET UP AND SOLVE MATRIX
       BB1(1,1:MNE1)=0.
       DO 110 J=1,NE
       DELTA(1,1,J:MNS)=AAA(1,1,J:MNS)*Y(1,1:MNS)
       DO 110 I=1,NS
 110   BB1(1,J:M1)=DELTA(1,I,J:M1)+BB1(1,J:M1)
C   (1) FREE ENERGY - GASEOUS SPECIES
       DO 170 I=1,NS
 170   YI1(1,I:M1)=Y(1,I:M1)/YBAR(1:M1)
       F(1,1:MNS)=VALOG(YI1(1,1:MNS):F(1,1:MNS))
```

```
      DO 180 I=1,NS
 180  F(1,I:M1)=Y(1,I:M1)*(FORT(1,I:M1)+F(1,I:M1))
C   INITIALIZE MATRICES
      A1(1,1,1:MX)=0.
      R1(1,1,1:MX)=0.
      A1(1,1,1:MNE)=BB1(1,1:MNE)
      DO 270 J=1,NE
      DO 270 K=1,J
      DELT(1,1:MNS)=AAA(1,1,J:MNS)*DELTA(1,1,K:MNS)
      DO 275 I=1,NS
 275  R1(1,J,K:M1)=DELT(1,I:M1)+R1(1,J,K:M1)
 270  R1(1,K,J:M1)=R1(1,J,K:M1)
      DO 280 J=2,MMM
      K=J-1
 280  A1(1,1,J:MNE)=R1(1,1,K:MNE)
      DO 310 J=2,MMM
      K=J-1
 310  A1(1,MMM,J:M1)=A1(1,K,1:M1)
      DO 320 J=1,NE
      DELT(1,1:MNS)=AAA(1,1,J:MNS)*F(1,1:MNS)
      BUM(1:M1)=0.
      DO 330 I=1,NS
 330  BUM(1:M1)=DELT(1,I:M1)+BUM(1:M1)
 320  BB1(1,J:M1)=BB1(1,J:M1)+BUM(1:M1)
      BUM(1:M1)=0.
      DO 340 I=1,NS
 340  BUM(1:M1)=BUM(1:M1)+F(1,I:M1)
      BB1(1,MMM:M1)=BUM(1:M1)
      CALL EQSOL(MMM,NE,M1)
C   NEW MOLE FRACTIONS (X)
      XYBAR(1:M1)=BB1(1,1:M1)
      BB1(1,1:MNE)=BB1(1,2:MNE)
      DELT(1,1:MNS)=0.
      DO 390 J=1,NE
      DO 400 I=1,NS
 400  DELT(1,I:M1)=DELT(1,I:M1)+AAA(1,I,J:M1)*BB1(1,J:M1)
 390  CONTINUE
      DO 410 I=1,NS
 410  DELT(1,I:M1)=DELT(1,I:M1)+XYBAR(1:M1)
      X(1,1:MNS)=DELT(1,1:MNS)*Y(1,1:MNS)-F(1,1:MNS)
      RETURN
      END
      SUBROUTINE EQSOL(MMM,NE,M1)
      COMMON/E7/A1(500,7,7),BB1(500,7)
      DIMENSION U(500,7),S(500),TK2(500),UT(500)
      DO 200 K=1,NE
```

```
      J=K
      S(1:M1)=0.
      DO 20 I=K,MMM
20    S(1:M1)=S(1:M1)+A1(1,I,J:M1)*A1(1,I,J:M1)
      S(1:M1)=VSQRT(S(1:M1):S(1:M1))
      U(1,K:M1)=A1(1,K,J:M1)+VSIGN(S(1:M1),A1(1,K,J:M1):UT(1:M1))
      KP1=K+1
      KM1=M1*(MMM-K)
      U(1,KP1:KM1)=A1(1,KP1,J:KM1)
      A1(1,K,J:M1)=-VSIGN(S(1:M1),A1(1,K,J:M1):UT(1:M1))
      TK2(1:M1)=U(1,K:M1)*S(1:M1)
      TK2(1:M1)=VABS(TK2(1:M1):TK2(1:M1))
      JK=K+1
      DO 70 JJ=JK,MMM
      UT(1:M1)=0.
      DO 50 III=K,MMM
 50   UT(1:M1)=UT(1:M1)+U(1,III:M1)*A1(1,III,JJ:M1)
      UT(1:M1)=UT(1:M1)/TK2(1:M1)
      DO 40 II=K,MMM
40    A1(1,II,JJ:M1)=A1(1,II,JJ:M1)-U(1,II:M1)*UT(1:M1)
70    CONTINUE
      UT(1:M1)=0.
      DO 80 II=K,MMM
80    UT(1:M1)=UT(1:M1)+U(1,II:M1)*BB1(1,II:M1)
      UT(1:M1)=UT(1:M1)/TK2(1:M1)
      DO 60 II=K,MMM
60    BB1(1,II:M1)=BB1(1,II:M1)-U(1,II:M1)*UT(1:M1)
200   CONTINUE
      BB1(1,7:M1)=BB1(1,7:M1)/A1(1,7,7:M1)
      BB1(1,6:M1)=(BB1(1,6:M1)-A1(1,6,7:M1)*BB1(1,7:M1))/A1(1,6,6:M1)
      BB1(1,5:M1)=(BB1(1,5:M1)-A1(1,5,7:M1)*BB1(1,7:M1)-A1(1,5,6:M1)*
     1BB1(1,6:M1))/A1(1,5,5:M1)
      BB1(1,4:M1)=(BB1(1,4:M1)-A1(1,4,7:M1)*BB1(1,7:M1)-A1(1,4,6:M1)*
     1BB1(1,6:M1)-A1(1,4,5:M1)*BB1(1,5:M1))/A1(1,4,4:M1)
      BB1(1,3:M1)=(BB1(1,3:M1)-A1(1,3,7:M1)*BB1(1,7:M1)-A1(1,3,6:M1)*
     1BB1(1,6:M1)-A1(1,3,5:M1)*BB1(1,5:M1)-A1(1,3,4:M1)*BB1(1,4:M1))/
     2A1(1,3,3:M1)
      BB1(1,2:M1)=(BB1(1,2:M1)-A1(1,2,7:M1)*BB1(1,7:M1)-A1(1,2,6:M1)*
     1BB1(1,6:M1)-A1(1,2,5:M1)*BB1(1,5:M1)-A1(1,2,4:M1)*BB1(1,4:M1)-
     2A1(1,2,3:M1)*BB1(1,3:M1))/A1(1,2,2:M1)
      BB1(1,1:M1)=(BB1(1,1:M1)-A1(1,1,7:M1)*BB1(1,7:M1)-A1(1,1,6:M1)*
     1BB1(1,6:M1)-A1(1,1,5:M1)*BB1(1,5:M1)-A1(1,1,4:M1)*BB1(1,4:M1)-
     2A1(1,1,3:M1)*BB1(1,3:M1)-A1(1,1,2:M1)*BB1(1,2:M1))/A1(1,1,1:M1)
      RETURN
      END
      SUBROUTINE TP(M1)
```

APPENDIX A

```
      DIMENSION B1(500),VISI(500,24),CONDI(500,24)
      COMMON/E1/T(500),P(500),WMIX(500),CL(500,6),SH(500)
      COMMON/E2/HI(500,24),MOLEF(500,24),CPI(500,24)
      COMMON/E4/MW(24),SYMB(24),AA(24,6),MWEL(6),AAA(500,24,6)
      COMMON/E5/FORT(500,24),Y(500,24),X(500,24),YBAR(500)
      COMMON/E8/NE,NS
      COMMON/E9/XMA(24),XMB(24),XMC(24),XKA(24),XKB(24)
      COMMON/E12/A9(500),A10(500),A13(500),AA1(500),AA2(500),TV1(500),
     1TV2(500)
      COMMON/E14/VIS(500),COND(500),SIG(500),CP(500)
      COMMON/E16/ENT(500,24),CPI1(500,24)
      EQUIVALENCE (VISI(1,1),ENT(1,1)),(CONDI(1,1),CPI1(1,1))
      BIT B1
      REAL MOLEF,MW
C     HERE VISI IS THE VISCOSITY OF SPECIF I.
      DO 200 I=1,NS
      VISI(1,I:M1)=(XMA(I)+XMB(I)*T(1:M1)+XMC(I)*T(1:M1)*T(1:M1))/.0672
      B1(1:M1)=VISI(1,I:M1).LE.0.
      VISI(1,I:M1)=Q8VCTRL(1.E-10,B1(1:M1):VISI(1,I:M1))
  200 CONTINUE
C     CP IS SPECIFIC HEAT OF MIXTURE.
      CP(1:M1)=0.
      DO 210 I=1,NS
      CP(1:M1)=CP(1:M1)+CPI(1,I:M1)*MOLEF(1,I:M1)
  210 CONTINUE
C     HERE CONDI IS THE THERMAL CONDUCTIVITY OF SPECIE I.
      DO 220 I=1,NS
      CONDI(1,I:M1)=(XKA(I)+XKB(I)*T(1:M1))/.0672
  220 CONTINUE
C     WILKE RELATION FOR MIXTURE VISCOSITY AND THERMAL CONDUCTIVITY.
      VIS(1:M1)=0.
      COND(1:M1)=0.
      DO 240 I=1,NS
      A13(1:M1)=0.
      DO 230 J=1,NS
      WJI1=MW(J)/MW(I)
      DENOM1=2.82*SQRT(1.+1./WJI1)
      WJI=SQRT(WJI1)
      WJI=SQRT(WJI)
      AA1(1:M1)=VISI(1,I:M1)/VISI(1,J:M1)
      AA1(1:M1)=VSQRT(AA1(1:M1):AA1(1:M1))
      AA1(1:M1)=1.+AA1(1:M1)*WJI
      AA1(1:M1)=AA1(1:M1)*AA1(1:M1)
      A13(1:M1)=A13(1:M1)+MOLEF(1,J:M1)*AA1(1:M1)/DENOM1
  230 CONTINUE
      VIS(1:M1)=MOLEF(1,I:M1)*VISI(1,I:M1)/A13(1:M1)+VIS(1:M1)
      COND(1:M1)=MOLEF(1,I:M1)*CONDI(1,I:M1)/A13(1:M1)+COND(1:M1)
  240 CONTINUE
C     PRANDTL NUMBER
      SIG(1:M1)=VIS(1:M1)*CP(1:M1)/COND(1:M1)/WMIX(1:M1)
      RETURN
      END
```

APPENDIX B

PROGRAM INPUT

The input for the present setup of the program EQUIL is given in this appendix.

```
&THERMO
 NS=24,NE=6,
MWEL(1)=5.486E-4,1.008,4.01,12.011,16.0,14.0,
MW(1)=5.486E-4,1.008,2.016,1.008,
 4.01,4.01,                     12.001,24.022,36.033,12.01,25.03,26.038,
   37.041,49.04,
                    16.,32.,16.,28.011,44.01,
                    14.,28.,14.,30.,30.,
&END
  E-        1
 0.2500000E+01 0.            0.            0.            0.               E       2
-0.7453750E+03-0.1173402E+02 GORDON AND MCBRIDE NASA SP-273               E       3
 0.2500000E+01 0.            0.            0.            0.               E       4
-0.7453749E+03-0.1173402E+02 GORDON AND MCBRIDE NASA SP-273               E       5
  0.2508E+01    -0.6332E-05    0.1364E-08    -0.1094E-12    0.2934E-17  E-      6
 -0.7450E+03    -0.1208E+02    ESCH ETAL NASA CR-111989                   E-      7
  0.0            .0500E-07    -.1000E-12     26.000E-05     0.0            E-   8
  H              1
 0.2500000E+01 0.            0.            0.            0.               H       2
 0.2547162E+05-0.4601176E+00 GORDON AND MCBRIDE NASA SP-273               H       3
 0.2500000E+01 0.            0.            0.            0.               H       4
 0.2547162E+05-0.4601176E+00 GORDON AND MCBRIDE NASA SP-273               H       5
 2.475164E+00  7.366387E-05 -2.537593E-08  2.386674E-12 -4.551431E-17     H       6
 2.523626E+04 -3.749137E-01 NICOLET NASA CR-132470                        H       7
  0.294E-05      .0889E-07    -.0811E-12      2.496E-05    5.1290E-08        H    8
  H2             2
 0.3057445E+01 0.2676520E-02-0.5809916E-05 0.5521039E-08-0.1812273E-11    H2      2
-0.9889047E+03-0.2299705E+01 GORDON AND MCBRIDE NASA SP-273               H2      3
 0.3100190E+01 0.5111946E-03 0.5264421E-07-0.3490997E-10 0.3694534E-14    H2      4
-0.8773804E+03-0.1962942E+01 GORDON AND MCBRIDE NASA SP-273               H2      5
  0.3363E+01     0.4656E-03   -0.5127E-07    0.2802E-11   -0.4905E-16     H2      6
 -0.1018E+04    -0.3716E+01    ESCH ETAL. NASA CR-111989                  H2      7
 -0.079E-05      .0791E-07    -.0886E-12      3.211E-05    5.3440E-08        H2   8
  H+        -1   1
 0.2500000E+01 0.            0.            0.            0.               H+      2
 0.1840334E+06-0.1153862E+01 GORDON AND MCBRIDE NASA SP-273               H+      3
 0.2500000E+01 0.            0.            0.            0.               H+      4
 0.1840334E+06-0.1153862E+01 GORDON AND MCBRIDE NASA SP-273               H+      5
 0.2500000E+01 0.            0.            0.            0.               H+      6
 0.1840334E+06-0.1153862E+01 GORDON AND MCBRIDE NASA SP-273               H+      7
  0.0            .0500E-07    -.1000E-12     26.000E-05     0.0             H+    8
  HE                  1
 0.2500000E+01 0.            0.            0.            0.               HE      2
-0.7453749E+03 0.9153488E+00 GORDON AND MCBRIDE NASA SP-273               HE      3
 0.2500000E+01 0.            0.            0.            0.               HE      4
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-0.7453749E+03 0.9153488E+00 GORDON AND MCBRIDE NASA SP-273              HE      5
 0.2500000E+01 0.            0.            0.            0.              HE      6
-0.7453749E+03 0.9153488E+00 GORDON AND MCBRIDE NASA SP-273              HE      7
   -1.3451E-06  2.311919E-08 -4.735988E-13    2.0388E-05    3.2493E-08    HE      8
   HE+      -1          1
 0.2500000E+01 0.            0.            0.            0.              HE+     2
 0.2853426E+06 0.1608404E+01 GORDON AND MCBRIDE NASA SP-273              HE+     3
 0.2500000E+01 0.            0.            0.            0.              HE+     4
 0.2853426E+06 0.1608404E+01 GORDON AND MCBRIDE NASA SP-273              HE+     5
 0.2500000E+01 0.            0.            0.            0.              HE+     6
 0.2853426E+06 0.1608404E+01 GORDON AND MCBRIDE NASA SP-273              HE+     7
    0.0            .0500E-07     -.1000E-12    26.000E-05    0.0            HE+  8
    C                        1                                                   1
 0.2532870E+01-0.1588764E-03 0.3068208E-06-0.2677006E-09 0.8748882E-13  C       2
 0.8524042E+05 0.4606237E+01 GORDON AND MCBRIDE NASA SP-273              C       3
 0.2581066E+01-0.1469620E-03 0.7438808E-07-0.7948107E-11 0.5890097E-16  C       4
 0.8521629E+05 0.4312887E+01 GORDON AND MCBRIDE NASA SP-273              C       5
    0.2141E+01     0.3219E-03    -0.5498E-07    0.3604E-11    -0.5564E-16  C       6
    0.8542E+05     0.6874E+01      ESCH ETAL NASA CR-111989                C       7
    1.997E-05       .1772E-07     -.3378E-12     2.506E-05      .7479E-08     C    8
   C2                        2                                                   1
 0.7451814E+01-0.1014468E-01 0.8587973E-05 0.8732110E-09-0.2442979E-11  C2      2
 0.9891198E+05-0.1584667E+02 GORDON AND MCBRIDE NASA SP-273              C2      3
 0.4043535E+01 0.2057365E-03 0.1090757E-06-0.3642787E-10 0.3412786E-14  C2      4
 0.9970948E+05 0.1277515E+01 GORDON AND MCBRIDE NASA SP-273              C2      5
    0.4026E+01     0.4857E-03    -0.7026E-07    0.4666E-11    -0.1142E-15  C2      6
    0.9787E+05     0.1090E+01 ESCH ETAL NASA CR-111989                     C2      7
    1.931E-05       .1393E-07     -.2575E-12      .859E-05      .6233E-08     C2   8
   C3                        3                                                   1
 0.5740846E+01-0.8428123E-02 0.1862019E-04-0.1451052E-07 0.3967697E-11  C3      2
 0.9715752E+05-0.2383737E+01 GORDON AND MCBRIDE NASA SP-273              C3      3
 0.3681536E+01 0.2416523E-02-0.8434811E-06 0.1450819E-09-0.9569730E-14  C3      4
 0.9741395E+05 0.6837780E+01 GORDON AND MCBRIDE NASA SP-273              C3      5
    0.2213E+02    -0.1759E-01     0.5565E-05    -0.6758E-09    0.2825E-13  C3      6
    0.9423E+05    -0.1021E+03 ESCH ETAL. NASA CR-111989                    C3      7
    2.019E-05       .1179E-07     -.1655E-12      .630E-05      .5804E-08     C3   8
   C+       -1               1
 0.2595384E+01-0.4068664E-03 0.6892366E-06-0.5266487E-09 0.1508337E-12  C+      2
 0.2166628E+06 0.3895729E+01 GORDON AND MCBRIDE NASA SP-273              C+      3
 0.2511827E+01-0.1735978E-04 0.9504267E-08-0.2218851E-11 0.1862189E-15  C+      4
 0.2166772E+06 0.4286129E+01 GORDON AND MCBRIDE NASA SP-273              C+      5
    0.2528E+01     0.4869E-05    -0.7026E-08    0.1134E-11    -0.3476E-16  C+      6
    0.2168E+06     0.4139E+01 ESCH ETAL. NASA CR-111989                    C+      7
    0.0            .0500E-07     -.1000E-12    26.000E-05    0.0            C+   8
   C2H                1      2
 0.2649940E+01 0.8491951E-02-0.9816537E-05 0.6537362E-08-0.1735627E-11  C2H     2
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0.5627575E+05 0.7689860E+01 GORDON AND MCBRIDE NASA SP-273            C2H     3
0.4420765E+01 0.2211930E-02-0.5929494E-06 0.9419577E-10-0.6852759E-14  C2H     4
0.5583544E+05-0.1158809E+01 GORDON AND MCBRIDE NASA SP-273
   0.5307E+01     0.8966E-03    -0.1378E-06     0.9251E-11    -0.2278E-15  C2H     6
   0.5809E+05    -0.5288E+01 ESCH ETAL. NASA CR-111989                  C2H     7
    2.404E-05      .1363E-07     -.2184E-12      1.126E-05      .7439E-08     C2H 8
C2H2               2             2
0.1410276E+01 0.1905727E-01-0.2450139E-04 0.1639087E-07-0.4134544E-11  C2H2    2
0.2618820E+05 0.1139382E+02 GORDON AND MCBRIDE NASA SP-273             C2H2    3
0.4575108E+01 0.5123835E-02-0.1745235E-05 0.2867306E-09-0.1795142E-13  C2H2    4
0.2560742E+05-0.3573794E+01 GORDON AND MCBRIDE NASA SP-273             C2H2    5
   0.6789E+01     0.1503E-02    -0.2295E-06     0.1534E-10    -0.3763E-15  C2H2    6
   0.2590E+05    -0.1539E+02 ESCH ETAL. NASA CR-111989                  C2H2    7
    1.396E-05      .0842E-07     -.6939E-12      1.126E-05      .7439E-08     C2H28
 C3H               1             3
3.3446607E+00 1.0687605E-02-1.3312138E-05 1.3389601E-08-5.6987727E-12  C3H     2
6.2581906E+04 6.0004184E+00 WAKELYN AND MCLAIN 72657                   C3H     3
3.8776821E+00 6.7242969E-03-2.6055734E-06 4.4163330E-10-2.7082704E-14  C3H     4
6.2564338E+04 3.8265297E+00 WAKELYN AND MCLAIN 72657                   C3H     5
3.8776821E+00 6.7242969E-03-2.6055734E-06 4.4163330E-10-2.7082704E-14  C3H     6
6.2564338E+04 3.8265297E+00 WAKELYN AND MCLAIN 72657                   C3H     7
    2.019E-05      .1179E-07     -.1655E-12       .630E-05      .5804E-08     C3H 8
 C4H               1             4
4.9686610E+00 1.7278593E-02-2.9943171E-05 3.2461613E-08-1.3663978E-11  C4H     2
7.5454605E+04-8.7699380E-01 WAKELYN AND MCLAIN 72657                   C4H     3
6.5312534E+00 6.5064621E-03-2.2517411E-06 3.3295782E-10-1.7214711E-14  C4H     4
7.5350412E+04-7.4467228E+00 WAKELYN AND MCLAIN 72657         214       C4H     5
6.5312534E+00 6.5064621E-03-2.2517411E-06 3.3295782E-10-1.7214711E-14  C4H     6
7.5350412E+04-7.4467228E+00 WAKELYN AND MCLAIN 72657         214       C4H     7
    2.019E-05      .1179E-07     -.1655E-12       .630E-05      .5804E-08     C4H 8
 O                             1                                               1
0.2946428E+01-0.1638166E-02 0.2421031E-05-0.1602843E-08 0.3890696E-12  O       2
0.2914764E+05 0.2963994E+01 GORDON AND MCBRIDE NASA SP-273             O       3
0.2542059E+01-0.2755061E-04-0.3102803E-08 0.4551067E-11-0.4368051E-15  O       4
0.2923080E+05 0.4920308E+01 GORDON AND MCBRIDE NASA SP-273             O       5
   0.2546E+01    -0.5952E-04     0.2701E-07    -0.2798E-11     0.9380E-16  O       6
   0.2915E+05     0.5049E+01 ESCH ETAL. NASA CR-111989                  O       7
    1.519E-05      .1875E-07     -.2228E-12      1.250E-05      .7092E-08       O 8
 O2                            2                                               1
0.3625598E+01-0.1878218E-02 0.7055454E-05-0.6763513E-08 0.2155599E-11  O2      2
-0.1047522E+04 0.4305277E+01 GORDON AND MCBRIDE NASA SP-273            O2      3
0.3621953E+01 0.7361826E-03-0.1965222E-06 0.3620155E-10-0.2894562E-14  O2      4
-0.1201982E+04 0.3615096E+01 GORDON AND MCBRIDE NASA SP-273            O2      5
   0.3721E+01     0.4254E-03    -0.2835E-07     0.6050E-12    -0.5186E-17  O2      6
  -0.1044E+04     0.3254E+01 ESCH ETAL. NASA CR-111989                  O2      7
    1.693E-05      .1496E-07     -.2276E-12      1.019E-05      .4901E-08      O2 8
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APPENDIX B

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  O+        -1                     1
0.2498479E+01 0.1141097E-04-0.2976139E-07 0.3224653E-10-0.1237551E-13  O+      2
0.1879490E+06 0.4386435E+01 GORDON AND MCBRIDE NASA SP-273             O+      3
0.2506048E+01-0.1446424E-04 0.1244604E-07-0.4685847E-11 0.6554887E-15  O+      4
0.1879470E+06 0.4347974E+01 GORDON AND MCBRIDE NASA SP-273             O+      5
   0.2944E+01    -0.4108E-03    0.9156E-07    -0.5848E-11    0.1190E-15  O+      6
   0.1879E+06     0.1750E+01 ESCH ETAL. NASA CR-111989                  O+      7
   0.0            .0500E-07    -.1000E-12    26.000E-05    0.0           O+  8
  CO                           1   1                                           1
0.3710092E+01-0.1619096E-02 0.3692359E-05-0.2031967E-08 0.2395334E-12  CO      2
-0.1435631E+05 0.2955535E+01 GORDON AND MCBRIDE NASA SP-273            CO      3
0.2984069E+01 0.1489139E-02-0.5789968E-06 0.1036457E-09-0.6935355E-14  CO      4
-0.1424522E+05 0.6347915E+01 GORDON AND MCBRIDE NASA SP-273            CO      5
   0.3366E+01     0.8027E-03    -0.1968E-06    0.1940E-10    -0.5549E-15  CO      6
  -0.1434E+05     0.4263E+01 ESCH ETAL. NASA CR-111989                  CO      7
   2.404E-05      .1363E-07    -.2184E-12      .859E-05      .6233E-08     CO  8
  CO2                          1   2                                           1
0.2400779E+01 0.8735095E-02-0.6607087E-05 0.2002186E-08 0.6327403E-15  CO2     2
-0.4837752E+05 0.9695145E+01 GORDON AND MCBRIDE NASA SP-273            CO2     3
0.4460804E+01 0.3098171E-02-0.1239257E-05 0.2274132E-09-0.1552595E-13  CO2     4
-0.4896144E+05-0.9863598E+00 GORDON AND MCBRIDE NASA SP-273            CO2     5
   0.4413E+01     0.3192E-02    -0.1298E-05    0.2415E-09    -0.1674E-13  CO2     6
  -0.4894E+05    -0.7288E+00 ESCH ETAL. NASA CR-111989                  CO2     7
   2.404E-05      .1363E-07    -.2184E-12      .859E-05      .6233E-08     CO  8
  N                                    1
0.2503071E+01-0.2180018E-04 0.5420528E-07-0.5647560E-10 0.2099904E-13  N       2
0.5609890E+05 0.4167576E+01 GORDON AND MCBRIDE NASA SP-273             N       3
0.2450268E+01 0.1066145E-03-0.7465337E-07 0.1879652E-10-0.1025983E-14  N       4
0.5611604E+05 0.4448758E+01 GORDON AND MCBRIDE NASA SP-273             N       5
   0.2748E+01    -0.3909E-03    0.1338E-06    -0.1191E-10    0.3369E-15  N       6
   0.5609E+05     0.2872E+01 ESCH ETAL. NASA CR-111989                  N       7
   0.253E-05      .2206E-07    -.3737E-12     1.281E-05      .8593E-08      N  8
  N2                                   2
0.3674826E+01-0.1208150E-02 0.2324010E-05-0.6321755E-09-0.2257725E-12  N2      2
-0.1061158E+04 0.2358042E+01 GORDON AND MCBRIDE NASA SP-273            N2      3
0.2896319E+01 0.1515486E-02-0.5723527E-06 0.9980739E-10-0.6522355E-14  N2      4
-0.9058618E+03 0.6161514E+01 GORDON AND MCBRIDE NASA SP-273            N2      5
   0.3727E+01     0.4684E-03    -0.1140E-06    0.1154E-10    -0.3293E-15  N2      6
  -0.1043E+04     0.1294E+01 ESCH ETAL. NASA CR-111989                  N2      7
   0.970E-05      .1613E-07    -.1916E-12      .654E-05      .6457E-08     N2  8
  N+        -1                         1
   0.2727E+01    -0.2820E-03    0.1105E-06    -0.1551E-10    0.7847E-15  N+      2
   0.2254E+06     0.3645E+01 ESCH ETAL. NASA CR-11989                   N+      3
   0.2727E+01    -0.2820E-03    0.1105E-06    -0.1551E-10    0.7847E-15  N+      4
   0.2254E+06     0.3645E+01 ESCH ETAL. NASA CR-111989                  N+      5
   0.2499E+01    -0.3725E-05    0.1147E-07    -0.1102E-11    0.3078E-16  N+      6
   0.2254E+06     0.4950E+01 ESCH ETAL. NASA CR-111989                  N+      7
   0.0            .0500E-07    -.1000E-12    26.000E-05    0.0            N+  8
  NO                               1   1
0.4045952E+01-0.3418178E-02 0.7981919E-05-0.6113931E-08 0.1591907E-11  NO      2
0.9745393E+04 0.2997499E+01 GORDON AND MCBRIDE NASA SP-273             NO      3
0.3189000E+01 0.1338228E-02-0.5289932E-06 0.9591933E-10-0.6484793E-14  NO      4
0.9828329E+04 0.6745813E+01 GORDON AND MCBRIDE NASA SP-273             NO      5
   0.3845E+01     0.2521E-03    -0.2658E-07    0.2162E-11    -0.6381E-16  NO      6
   0.9764E+04     0.3212E+01 ESCH ETAL. NASA CR-111989                  NO      7
   0.970E-05      .1613E-07    -.1916E-12      .654E-05      .6457E-08      NO  8
  NO+       -1                     1   1
0.3668506E+01-0.1154458E-02 0.2175561E-05-0.4822747E-09-0.2784791E-12  NO+     2
0.1180337E+06 0.3177932E+01 GORDON AND MCBRIDE NASA SP-273             NO+     3
0.2888549E+01 0.1521712E-02-0.5753124E-06 0.1005108E-09-0.6604429E-14  NO+     4
0.1181924E+06 0.7002720E+01 GORDON AND MCBRIDE NASA SP-273             NO+     5
0.2888549E+01 0.1521712E-02-0.5753124E-06 0.1005108E-09-0.6604429E-14  NO+     6
0.1181924E+06 0.7002720E+01 GORDON AND MCBRIDE NASA SP-273             NO+     7
   0.970E-05      .1613E-07    -.19165-12      .654E-05      .6457E-08     NO+ 8
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TABLE I.- NAMELIST THERMO

Variable	Definition
NS	Number of species present in the mixture; NS = 24
NE	Number of elements present in the mixture, including electrons; NE = 6
MWEL	An array of molecular weights of the elements present
MW	An array of molecular weights of the species present

TABLE II.- ELEMENTAL PARTICLES TABLE

Species (i)	Values for AA(i,j) array using element (j) -					
	e^-	H	He	C	O	N
e^-	1.	0.	0.	0.	0.	0.
H	0.	1.	0.	0.	0.	0.
H_2	0.	2.	0.	0.	0.	0.
H^+	-1.	1.	0.	0.	0.	0.
He	0.	0.	1.	0.	0.	0.
He^+	-1.	0.	1.	0.	0.	0.
C	0.	0.	0.	1.	0.	0.
C_2	0.	0.	0.	2.	0.	0.
C_3	0.	0.	0.	3.	0.	0.
C^+	-1.	0.	0.	1.	0.	0.
C_2H	0.	1.	0.	2.	0.	0.
C_2H_2	0.	2.	0.	2.	0.	0.
C_3H	0.	1.	0.	3.	0.	0.
C_4H	0.	1.	0.	4.	0.	0.
O	0.	0.	0.	0.	1.	0.
O_2	0.	0.	0.	0.	2.	0.
O^+	-1.	0.	0.	0.	1.	0.
CO	0.	0.	0.	1.	1.	0.
CO_2	0.	0.	0.	1.	2.	0.
N	0.	0.	0.	0.	0.	1.
N_2	0.	0.	0.	0.	0.	2.
N^+	-1.	0.	0.	0.	0.	1.
NO	0.	0.	0.	0.	1.	1.
NO^+	-1.	0.	0.	0.	1.	1.

TABLE III.- RESULTS FOR FIRST EXAMPLE

Species (i)	Mole fractions for mesh point -		
	1	101	201
e^-	.10356E-10	.65454E-04	.55216E-01
H	.41791E+00	.85288E+00	.78588E+00
H_2	.44188E+00	.16587E-01	.10254E-03
H^+	.10030E-06	.59900E-05	.33278E-01
He	.81824E-01	.53100E-01	.49085E-01
He^+	.11205E-20	.89638E-15	.33561E-06
C	.23667E-02	.71937E-01	.51611E-01
C_2	.71464E-03	.17929E-02	.14203E-05
C_3	.94738E-03	.22540E-04	.98840E-11
C^+	.65849E-06	.60351E-04	.21840E-01
C_2H	.25102E-01	.31818E-03	.10560E-08
C_2H_2	.14824E-01	.30029E-05	.24556E-13
C_3H	.68313E-02	.34229E-05	.13116E-14
C_4H	.26219E-02	.11006E-06	.66449E-18
O	.47058E-07	.67763E-04	.28840E-02
O_2	.67916E-15	.11418E-10	.51267E-09
O^+	.97430E-14	.10728E-08	.98447E-04
CO	.49752E-02	.31593E-02	.66140E-06
CO_2	.20416E-09	.75944E-09	.53915E-14
N	.10220E-05	.18098E-05	.15684E-05
N_2	.21336E-05	.36198E-09	.57447E-14
N^+	.72752E-13	.93510E-11	.10534E-06
NO	.26104E-10	.11051E-09	.26882E-11
NO^+	.89366E-12	.19795E-11	.90302E-12

TABLE III.- Concluded

Thermodynamic and transport quantities for the mixture	Mesh point 1	Mesh point 101	Mesh point 201
Enthalpy, J/kg	.68375E+08	.17007E+09	.28681E+09
Specific heat, J/kg-K	.97937E+04	.10073E+05	.12513E+05
Viscosity, N-sec/m^2	.67567E-04	.11113E-03	.17887E-03
Conductivity, W/m-K	.13222E+01	.18599E+01	.34679E+01
Prandtl number	.50052E+00	.60192E+00	.64548E+00
Mixture molecular weight	.32553E+01	.21118E+01	.19523E+01

TABLE IV.- RESULTS FOR SECOND EXAMPLE

Species (i)	Mole fractions for mesh point -		
	1	101	201
e^-	.51200E-03	.17932E-03	.76507E-06
H	.10608E-03	.12973E-03	.14546E-03
H_2	.63731E-10	.31662E-10	.78930E-08
H^+	.52121E-08	.16868E-08	.97069E-10
He	.24459E-04	.29650E-04	.33909E-04
He^+	.30139E-14	.10362E-20	.12286E-23
C	.22278E-04	.54805E-06	.22217E-10
C_2	.25186E-11	.17195E-12	.33864E-19
C_3	.64357E-23	.51556E-21	.13274E-25
C^+	.36922E-06	.19954E-08	.25887E-13
C_2H	.31134E-18	.16576E-22	.74580E-23
C_2H_2	.18587E-27	.11607E-24	.57230E-25
C_3H	.33961E-23	.38821E-25	.50137E-29
C_4H	.21375E-30	.37541E-32	.20308E-40
O	.26123E+00	.31168E+00	.25236E+00
O_2	.33795E-04	.24698E-03	.34585E-01
O^+	.53787E-04	.36374E-05	.49716E-09
CO	.25821E-04	.61045E-04	.61969E-04
CO_2	.81239E-09	.10493E-07	.89826E-06
N	.47790E+00	.16095E+00	.13023E-02
N_2	.25688E+00	.51837E+00	.66646E+00
N^+	.12045E-03	.16831E-05	.11455E-09
NO	.27366E-02	.81706E-02	.45044E-01
NO^+	.34498E-03	.18364E-03	.12500E-04

TABLE IV.- Concluded

Thermodynamic and transport quantities for the mixture	Mesh point 1	Mesh point 101	Mesh point 201
Enthalpy, J/kg	.25612E+08	.14583E+08	.73277E+07
Specific heat, J/kg-K	.15926E+04	.13997E+04	.13339E+04
Viscosity, N-sec/m^2	.19216E-03	.15987E-03	.11002E-03
Conductivity, W/m-K	.39288E+00	.31231E+00	.21043E+00
Prandtl number	.77901E+00	.71658E+00	.69747E+00
Mixture molecular weight	.18160E+02	.22015E+02	.25177E+02

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Ajay Kumar: Research Associate Professor, Old Dominion University Research Foundation, Norfolk, Virginia.

16. Abstract

A vectorized code, EQUIL, is developed for calculating the equilibrium chemistry of a reacting gas mixture on the Control Data STAR-100 computer. The code provides species mole fractions, mass fractions, and thermodynamic and transport properties of the mixture for given temperature, pressure, and elemental mass fractions. The code is set up for the e^-, H, He, C, O, N system of elements. In all, 24 chemical species are included.

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